

Extended Quantum XOR Gate in Terms of Two-Spin Interactions

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ABSTRACT

Considerations of feasibility of quantum computing lead to the study of multispin quantum gates in which the input and output two-state systems (spins) are not identical. We provide a general discussion of this approach and then propose an explicit *two-spin interaction* Hamiltonian which accomplishes the quantum XOR gate function for a system of three spins: two input and one output.

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The size of semiconductor computer components is still quite far from atomic dimensions. They will soon reach [1] linear dimensions of about $0.25\text{ }\mu\text{m}$. This is $2500\text{ }\text{\AA}$, well above the sizes at which quantum-mechanical effects will be important. It has become clear, however, that as the miniaturization continues, atomic dimensions will be reached, perhaps, with technology different from today's semiconductors. Then, quantum-mechanical effects will have to be considered in computer operation. Lead by this expectation, some early works [2-4] considered how quantum mechanics affects the foundations of computer science. Questions such as limitations on “classical” computation due to quantum fluctuations, etc., have been raised.

A more “active” approach, initiated recently by many authors [4-30] is to attempt to harness the quantum nature of components of atomic dimensions for more efficient computation and design. This ambitious program involves many interesting scientific concepts new to both Computer Science and Physics. In order to answer whether quantum computation is feasible and useful, several issues must be addressed. Is quantum computation faster than classical computation? Can quantum computational elements be built and combined with other quantum and/or classical components? What will be the “design” rules for quantum computer components in order to perform Boolean logic operations on quantum bits (qubits) such as the up and down spin states of a spin- $\frac{1}{2}$ particle?

What are the error correction requirements and methods in quantum computation?

The answers to some of the questions that result from consideration of these general issues are still in the future. However, many definitive results have already been obtained. Specifically, on the theoretical side, new fast quantum algorithms have been proposed [31-35]. Error correction techniques [10,27,31,36,37], unitary operations corresponding to the simplest logic gates [5-30], and some Hamiltonians for gate operation [10,14,24,28-30] have been explored. Ideas on how to combine the simplest quantum gates have been put forth, e.g., [7,15,38]. On the side of experiment, there are several atomic-scale systems where the simplest quantum-gate functions have been recently realized [26,39,40] or contemplated [19].

There are, however, many general [4,18] and specific problems both with theory and experimental realizations of quantum computing. Just to mention one of them, the reversibility of coherent quantum evolution implies that the time scale Δt of the operation of quantum logic gates must be built into the Hamiltonian. As a result, virtually all proposals available to date assume that computation will be externally timed, i.e., interactions will be switched “on” and “off,” for instance, by laser radiation.

Thus, while we deem it inevitable that quantum properties of matter on the atomic scale will have to be considered in computer component design and use, we recognize that it is still a long way to go, with modern technology, to a really “desktop” fully coherent quantum computational unit. We propose to adopt a more realistic expectation that technological advances will first allow design and manufacturing of limited-size units, based on several tens of atomic two-level systems, operating in a quantum-coherent fashion over a large time interval and possibly driven externally by laser beams. These units will then become parts of a larger “classical” computer which will not maintain a quantum-coherent operation over its macroscopic dimensions.

A program of study should therefore begin with the simplest quantum logic gates in order to identify which Hamiltonians are typical for interactions required for their operation. Results presently available are limited; they include Hamiltonians for certain NOT [14,28] and controlled-NOT gates [10,30], and for some copying processes [29,30], as well as general analyses of possibility of construction of quantum operations [8,22]. In order to make connections with the present “classical” computer-circuitry design rules and have a natural way of identifying, at least initially, which multi-qubit systems are of interest, we propose to consider spatially extended quantum gates, i.e., gates with input and output qubits different.

Of course, reversibility of coherent quantum evolution makes the distinction between the input and output less important than in irreversible present-day computer components. However, we consider this notion useful within our general goals: to learn what kind of interactions are involved and to consider also units that might be connected to/as in “classical” computer devices. While our present study is analytical, we foresee studies of systems of order 20 to 25 two-state (qubit) atomic “components” with general-parameter interactions identified in the earlier work. Then, by using ordinary computers one can design those interaction values for which the resulting computational units will be useful as part of a computer and will be usable for Boolean logic operations (this need of numerical calculations limits the number of constituents to 20-25, i.e., to systems with total of 2^{20} to 2^{25} states that modern “classical” computers can handle).

A more futuristic goal of incorporating such computational units in actual computer design will require a whole new branch of computer engineering because the “built-in” Boolean functions will be quite complicated as compared to the present-day components such as NOT, AND, OR, NAND, to which computer designers are accustomed. Furthermore, the rules of their interconnection with each other and with the rest of the “classical” computer will be different from today’s devices.

In this Letter we consider the XOR gate. Let us use the term “spin” to describe a two-state system, and we will represent spin- $\frac{1}{2}$ -particle spin-components (measured in units of $\hbar/2$) by the standard Pauli matrices $\sigma_{x,y,z}$. In Figure 1, we denote by A , B , C the three two-state systems, i.e., three spins, involved. We assume that at time t the input spins A and B are in one of the basis states $|AB\rangle = |11\rangle, |10\rangle, |01\rangle$, or $|00\rangle$, where 1 and 0 denote the eigenstates of the z -component of the spin operator, with 1 referring to the “up” state and 0 referring to the “down” state. We use this notation for consistency with the classical “bit” notion. The initial state of C is not specified (it is arbitrary).

We would like to have a quantum evolution which, provided A and B are initially in those basis states, mimics the truth table of XOR:

A	B	output
1	1	0
1	0	1
0	1	1
0	0	0

(1)

were the output is at time $t + \Delta t$. One way to accomplish this is to produce the output in A or B , i.e., work with a two-spin system where the input and output are the same. The Hamiltonian for such a system is not unique. Explicit examples can be found in [10,30] where XOR was obtained as a sub-result of the controlled-NOT gate operation. In this case of two spins involved, the interactions can be single- and two-spin

only.

An important question is whether multispin systems can produce useful logical operations with only two-spin interactions. Indeed, two-particle interactions are much better studied and accessible to experimental probe than multiparticle interactions. Here we report such an example for the three-spin system depicted in Figure 1. To our best knowledge, this is the first such result in the literature.

Thus, we require that the XOR result will be generated in C at time $t + \Delta t$. The final states of A and B , as well as the *phase* of C are not really specified (they are arbitrary). In fact, there are many different unitary transformations, U , that correspond to the desired evolution in the eight-state space with the basis $|ABC\rangle = |111\rangle, |110\rangle, |101\rangle, |100\rangle, |011\rangle, |010\rangle, |001\rangle, |000\rangle$, which we will use in this order. The choice of the transformation determines what happens when the initial state is a superposition of the reference states, what are the phases in the output, etc. The transformation is definitely not unique.

Consider the following Hamiltonian,

$$H = \frac{\pi\hbar}{4\Delta t} \left(\sqrt{2}\sigma_{zA}\sigma_{yB} + \sqrt{2}\sigma_{zB}\sigma_{yC} - \sigma_{yB}\sigma_{xC} \right) \quad (2)$$

It is written here in terms of the spin components. In the eight-state

basis specified earlier, its matrix can be obtained by direct product of the Pauli matrices and unit 2×2 matrices \mathcal{I} . Here the subscripts A, B, C denote the spins. For instance, the first interaction term is proportional to

$$\sigma_{zA} \otimes \sigma_{yB} \otimes \mathcal{I}_C \quad (3)$$

etc. This Hamiltonian involves only two-spin-component interactions. In fact, A and C only interact with B , see Figure 1, so diagrammatically there is no loop (it is not known if the latter property is significant since we are dealing here with “nonequilibrium,” i.e., non-ground-state, calculations).

One can show that the Hamiltonian (2) corresponds to the XOR result in C at $t + \Delta t$ provided A and B where in one of the allowed superpositions of the appropriate “binary” states at t (we refer to superposition here because C is arbitrary at t). There are two ways to verify this claim. Firstly, one can diagonalize H directly, calculate U in the diagonal representation by using the general relation (valid for Hamiltonians which are constant during the time interval Δt ; see [28] for a formulation that introduces a multiplicative time dependence in H),

$$U = \exp(-iH\Delta t/\hbar) \quad (4)$$

and then reverse the diagonalizing transformation. The result for U , as a matrix in the basis selected earlier, is

$$U = \begin{pmatrix} 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix} \quad (5)$$

The calculation is extremely cumbersome (it was carried out, in part, by using Maple symbolic computer language); we do not reproduce it here.

The second, more general approach, by which the form (2) was actually obtained originally, is to analyze generally 8×8 unitary matrices corresponding to the XOR evolution, i.e., any linear combination of the states $|\underline{11}1\rangle$ and $|\underline{11}0\rangle$ evolves into a linear combination of $|\underline{11}0\rangle$, $|\underline{10}0\rangle$, $|\underline{01}0\rangle$, and $|\underline{00}0\rangle$, compare the underlined quantum numbers with the first entry in (1), with similar rules for the other three entries in (1). One can conjecture and analyze forms that yield two-spin interaction Hamiltonians. This approach is also quite cumbersome and not particularly illuminating. It will be detailed elsewhere [41]; the result is a three-parameter family of two-spin XOR Hamiltonians [41] from which we selected (2) as a particularly elegant and short (and also “loopless” in the sense mentioned earlier) form.

It is quite straightforward to check that, with phase factors -1 in some cases, the unitary matrix U indeed places the $\text{XOR}(A, B)$ in C . Note that (2) is not symmetric in A and B , so that another Hamiltonian can be obtained by relabeling.

In summary, we demonstrated by explicit example that two-spin interaction Hamiltonians can be useful in generating standard logical operations in systems with more than two spins. Analytical results and general rules are difficult to come up with. It is likely that future quantum logic gate “design” will involve heavy numerical simulations of systems of several spins with trial two-spin interactions, to determine interaction parameter values for which they perform useful logical operations.

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FIGURE CAPTION

Figure 1: Three two-state systems (spins) A , B , C , with the pairwise spin-component interactions in (2) marked schematically by the connecting lines. The XOR operation accomplished by (2) in time Δt assumes that A and B are the input qubits and C is the output qubit.